

gas phase

Ru1	0.7440850	0.2975150	0.0451600
Cl2	3.0869240	0.9991460	0.1048890
C3	0.3251590	2.3283300	0.0055970
N4	0.2889370	3.2765140	0.9784280
N5	0.2973320	2.9726620	-1.1921200
C6	0.3700140	4.6539680	0.4438530
H7	-0.4279770	5.2763540	0.8603800
H8	1.3309740	5.1028090	0.7182090
C9	0.2374740	4.4423380	-1.0705060
H10	1.0508350	4.9077980	-1.6343040
H11	-0.7117490	4.8183250	-1.4720320
Cl12	0.7658710	-0.0024210	1.8438150
Cl13	1.4839260	-1.7867120	-0.9349710
C14	0.1051090	3.1067890	2.3931750
C15	-0.3318650	2.8803360	5.1613870
C16	1.2093290	3.1008760	3.2673230
C17	-1.2141170	3.0860290	2.8934200
C18	-1.4081440	2.9615090	4.2722080
C19	0.9610370	2.9689180	4.6394010
H20	-2.4244040	2.9344450	4.6601290
H21	1.8104550	2.9455350	5.3186310
C22	0.1034360	2.3674690	-2.4840300
C23	-0.3359290	1.3044910	-5.0473110
C24	-1.2109360	2.0558660	-2.8940710
C25	1.1940610	2.2161600	-3.3643830
C26	0.9455440	1.6694410	-4.6291290
C27	-1.4038020	1.5209740	-4.1705550
H28	1.7844940	1.5324960	-5.3072770
H29	-2.4147260	1.2759010	-4.4897730
C30	2.5897850	2.6478500	-2.9917220
H31	2.9200980	2.1806960	-2.0586600
H32	2.6462980	3.7357180	-2.8563040
H33	3.2943870	2.3795400	-3.7830740
C34	-2.4030360	2.3039390	-1.9979300
H35	-3.3301250	2.0323740	-2.5096270
H36	-2.4836170	3.3576390	-1.7071950
H37	-2.3446220	1.7175140	-1.0771120
C38	-0.5622070	0.6850610	-6.4066620
H39	-0.4195070	-0.4020910	-6.3700640
H40	0.1402640	1.0774580	-7.1483860
H41	-1.5786200	0.8697900	-6.7680050
C42	2.6223920	3.2775460	2.7717960
H43	3.3386850	3.0449270	3.5646730
H44	2.7998860	4.3189860	2.4717320
H45	2.8411680	2.6408420	1.9094440
C46	-2.4097720	3.2390240	1.9790720
H47	-2.4820760	4.2600750	1.5829830
H48	-3.3385420	3.0369480	2.5198370
H49	-2.3631580	2.5678190	1.1181200

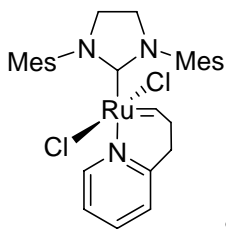
C50	-0.5600630	2.6976920	6.6440680
H51	0.2175370	3.1937620	7.2330650
H52	-0.5443490	1.6349720	6.9181520
H53	-1.5300660	3.0988660	6.9532730
H54	1.7266630	0.1608270	2.3466540
N55	-1.2236780	-0.5855980	-0.1702200
C56	-3.5275140	-2.0941990	-0.6709120
C57	-1.5318170	-1.0072280	-1.4173550
C58	-2.0524110	-0.9192720	0.8454920
C59	-3.2057250	-1.6772840	0.6157980
C60	-2.6707760	-1.7444610	-1.7111970
H61	-0.8247770	-0.7470050	-2.1933260
H62	-3.8401930	-1.9341710	1.4582490
H63	-2.8609790	-2.0484270	-2.7348900
H64	-4.4210250	-2.6840480	-0.8546610
C65	-1.7321570	-0.4376310	2.2366020
H66	-2.4135210	-0.9282930	2.9396220
H67	-1.9445390	0.6348540	2.2922040
C68	-0.2839010	-0.6510060	2.6914520
H69	-0.0476230	-1.7277210	2.7322630
H70	-0.1844330	-0.2815790	3.7219170

	U	Cv	S	H	G
trans.	0.889	2.981	45.045	1.481	-11.949
rot.	0.889	2.981	37.053	0.889	-10.159
vib.	19.014	121.139	121.457	19.014	-17.198
elec.	0.000	0.000	0.000	0.000	0.000
total	20.791	127.101	203.555	21.384	-39.306

Total internal energy, Utot (SCFE + ZPE + U): -2304.174882 hartrees

Total enthalpy, Htot (Utot + pV): -2304.173938 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -2304.270653 hartrees



gas phase

Ru1	0.5158900	0.2951250	0.0494930
Cl2	2.8961680	0.6220360	-0.4387890
C3	0.1847950	2.3607580	-0.0088600
N4	0.0355770	3.2782790	0.9758150
N5	0.0546370	3.0145760	-1.1941800
C6	-0.2521290	4.6451980	0.4734330
H7	-1.2483660	4.9626070	0.7996130
H8	0.4759340	5.3600450	0.8689130
C9	-0.1544980	4.4735420	-1.0489060
H10	0.6893020	5.0213420	-1.4814090
H11	-1.0646860	4.7860200	-1.5693260
C12	0.7850120	0.0567340	1.8405770

C13	0.1257810	3.0878420	2.3961400
C14	0.3117390	2.8325380	5.1874740
C15	1.3690980	3.2933330	3.0303100
C16	-1.0288010	2.7850510	3.1378900
C17	-0.9085080	2.6559840	4.5290930
C18	1.4386960	3.1561890	4.4199510
H19	-1.7970170	2.4151260	5.1100030
H20	2.3973260	3.3049450	4.9148030
C21	0.1949460	2.4426900	-2.5093420
C22	0.4587590	1.3137880	-5.0750550
C23	-0.9542090	1.9800540	-3.1901670
C24	1.4482980	2.4672290	-3.1547810
C25	1.5569980	1.8782700	-4.4215090
C26	-0.7928150	1.4029170	-4.4539450
H27	2.5291270	1.8747800	-4.9116650
H28	-1.6739550	1.0293710	-4.9731000
C29	2.6407280	3.1903020	-2.5754950
H30	3.5748120	2.7552080	-2.9395530
H31	2.6564480	3.1527720	-1.4881390
H32	2.6281950	4.2431680	-2.8880870
C33	-2.3424150	2.1790450	-2.6290870
H34	-3.0851030	1.6815260	-3.2583220
H35	-2.5992190	3.2453230	-2.6027890
H36	-2.4333960	1.7845290	-1.6166560
C37	0.6059400	0.6429630	-6.4213250
H38	0.6285380	-0.4493730	-6.3164020
H39	1.5312600	0.9441780	-6.9213600
H40	-0.2347170	0.8826590	-7.0814480
C41	2.6101620	3.6230240	2.2327220
H42	3.4756360	3.7226860	2.8940320
H43	2.5031840	4.5653870	1.6818460
H44	2.8296180	2.8427090	1.4943150
C45	-2.3705550	2.6004000	2.4698990
H46	-2.6924140	3.5138800	1.9549280
H47	-3.1361940	2.3508650	3.2104550
H48	-2.3378420	1.8014350	1.7218370
C49	0.4231240	2.6792710	6.6881210
H50	0.9198050	3.5451530	7.1411300
H51	1.0179910	1.7961150	6.9539490
H52	-0.5605080	2.5709270	7.1545040
H53	1.3108320	0.8279000	2.4116390
N54	0.8465910	-1.8852650	-0.2207210
C55	1.2416880	-4.5960800	-0.7489200
C56	1.4233310	-2.2925790	-1.3688880
C57	0.4598930	-2.8115950	0.6837780
C58	0.6560740	-4.1763730	0.4423450
C59	1.6326000	-3.6313650	-1.6780790
H60	1.7382910	-1.5053660	-2.0458460
H61	0.3442730	-4.8969730	1.1931890
H62	2.0988910	-3.9039300	-2.6198580
H63	1.3949450	-5.6537510	-0.9468350
C64	-0.2144820	-2.3350430	1.9468700
H65	-0.3027620	-3.1756080	2.6426390
H66	-1.2286240	-2.0159810	1.6843060
C67	0.5022150	-1.1716880	2.6446620
H68	1.4675310	-1.5071110	3.0617890
H69	-0.0838700	-0.8615810	3.5245800

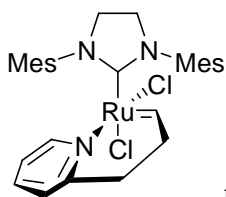
C170 -1.8854550 -0.1634400 -0.0940420

	U	Cv	S	H	G
	-----	-----	-----	-----	-----
trans.	.889	2.981	45.045	1.481	-11.949
rot.	.889	2.981	37.216	.889	-10.207
vib.	18.722	120.334	119.702	18.722	-16.968
elec.	.000	.000	.000	.000	.000
total	20.499	126.296	201.963	21.092	-39.124

Total internal energy, Utot (SCFE + ZPE + U): -2304.187193 hartrees

Total enthalpy, Htot (Utot + pV): -2304.186249 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -2304.282209 hartrees



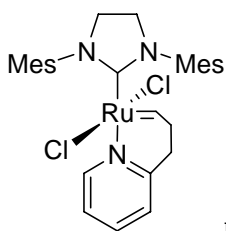
methylene chloride

Ru1	0.6364020	0.2868660	0.0419300
Cl2	3.0310740	0.8817430	-0.0081470
C3	0.2908930	2.3338880	-0.0385240
N4	0.2677630	3.2723310	0.9381320
N5	0.2771950	2.9774140	-1.2336690
C6	0.3291840	4.6587420	0.4105320
H7	-0.4862090	5.2615840	0.8205080
H8	1.2768990	5.1247780	0.6995130
C9	0.2172950	4.4523750	-1.1064290
H10	1.0394050	4.9182480	-1.6563070
H11	-0.7251440	4.8286690	-1.5197340
Cl2	0.6982300	0.0724170	1.8542210
Cl13	1.2846600	-1.9773110	-0.7105100
C14	0.1259730	3.0852320	2.3554770
C15	-0.2142060	2.8171430	5.1338660
C16	1.2575430	3.0978480	3.1947980
C17	-1.1762430	3.0225760	2.8954860
C18	-1.3217610	2.8770390	4.2791330
C19	1.0603070	2.9454850	4.5732270
H20	-2.3244430	2.8167560	4.6989200
H21	1.9320310	2.9362100	5.2253380
C22	0.1496730	2.3760760	-2.5353790
C23	-0.1496320	1.3172240	-5.1255560
C24	-1.1368360	2.0280010	-3.0033760
C25	1.2756570	2.2783120	-3.3797730
C26	1.1002560	1.7317020	-4.6572360
C27	-1.2585770	1.4890800	-4.2886680
H28	1.9689310	1.6393660	-5.3068740
H29	-2.2474070	1.2139650	-4.6508790
C30	2.6308390	2.8049870	-2.9752150
H31	2.8815780	2.5284240	-1.9494380
H32	2.6620080	3.9001470	-3.0521990
H33	3.4075000	2.4127410	-3.6383900
C34	-2.3764050	2.2812170	-2.1743510

H35	-3.2592670	1.8616940	-2.6643080
H36	-2.5519360	3.3564490	-2.0441800
H37	-2.3038590	1.8419930	-1.1766720
C38	-0.2976360	0.7050810	-6.4994340
H39	-0.1648560	-0.3835810	-6.4604500
H40	0.4524100	1.0968990	-7.1939630
H41	-1.2901230	0.8963560	-6.9198140
C42	2.6509010	3.3126210	2.6561780
H43	3.3981750	3.0538790	3.4122890
H44	2.8078620	4.3670900	2.3921040
H45	2.8415450	2.7140200	1.7619120
C46	-2.4009720	3.1518200	2.0168190
H47	-2.4991330	4.1694840	1.6181760
H48	-3.3097600	2.9359570	2.5855630
H49	-2.3663370	2.4756970	1.1579640
C50	-0.3901920	2.6130520	6.6213170
H51	0.4193210	3.0836640	7.1882940
H52	-0.3843250	1.5445780	6.8738950
H53	-1.3415580	3.0248310	6.9730490
H54	1.6534330	0.3128800	2.3371090
N55	-1.3499580	-0.5389910	-0.0950030
C56	-3.6397120	-2.0859860	-0.5439300
C57	-1.7116740	-0.9202180	-1.3416200
C58	-2.1217420	-0.9269960	0.9476110
C59	-3.2677400	-1.7051440	0.7408020
C60	-2.8425350	-1.6765430	-1.6122460
H61	-1.0558400	-0.6059990	-2.1443960
H62	-3.8573800	-2.0079190	1.6010650
H63	-3.0748380	-1.9493490	-2.6368600
H64	-4.5257750	-2.6937670	-0.7067120
C65	-1.7667820	-0.4806090	2.3430370
H66	-2.3799450	-1.0450100	3.0523070
H67	-2.0578120	0.5691960	2.4523540
C68	-0.2924800	-0.6050780	2.7420040
H69	0.0075800	-1.6667020	2.7855280
H70	-0.1714720	-0.2279870	3.7668510

	U	Cv	S	H	G
	-----	-----	-----	-----	-----
trans.	0.933	2.981	45.289	1.556	-12.626
rot.	0.933	2.981	37.221	0.933	-10.722
vib.	20.656	126.151	125.644	20.656	-18.689
elec.	0.000	0.000	0.000	0.000	0.000
total	22.523	132.112	208.154	23.146	-42.038

Total internal energy, Utot (SCFE + ZPE + U): -2304.260207 hartrees
Total enthalpy, Htot (Utot + pV): -2304.259216 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2304.363092 hartrees



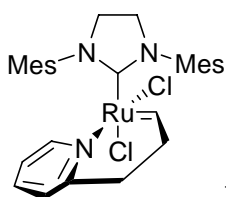
methylene chloride

Ru1	0.5405820	0.3074850	0.0588370
Cl2	2.9543770	0.6437320	-0.2451760
C3	0.2005160	2.3696420	-0.0045970
N4	0.0666890	3.2951330	0.9739060
N5	0.0557290	3.0132160	-1.1928080
C6	-0.2082680	4.6617290	0.4652950
H7	-1.1823450	5.0081550	0.8263250
H8	0.5526210	5.3624090	0.8231640
C9	-0.1729900	4.4696420	-1.0577490
H10	0.6394970	5.0270410	-1.5356730
H11	-1.1124430	4.7560150	-1.5407750
C12	0.7043580	0.0398660	1.8580810
C13	0.1456480	3.1045590	2.3938260
C14	0.3003730	2.8355230	5.1840160
C15	1.3800720	3.3136370	3.0416330
C16	-1.0166460	2.7914370	3.1206650
C17	-0.9124360	2.6564250	4.5116700
C18	1.4329480	3.1712550	4.4317440
H19	-1.8063510	2.4089290	5.0816540
H20	2.3846050	3.3244550	4.9382730
C21	0.1664290	2.4286340	-2.5039290
C22	0.3739060	1.2730750	-5.0611770
C23	-1.0017580	2.0048680	-3.1740100
C24	1.4181430	2.3992500	-3.1548260
C25	1.4981560	1.7976100	-4.4164030
C26	-0.8690200	1.4144600	-4.4357450
H27	2.4662140	1.7542490	-4.9125400
H28	-1.7662670	1.0686280	-4.9467420
C29	2.6356970	3.0874220	-2.5846360
H30	3.5522700	2.6643590	-3.0051220
H31	2.6924890	2.9965590	-1.5010030
H32	2.6193880	4.1551740	-2.8446260
C33	-2.3797720	2.2606510	-2.6122610
H34	-3.1243440	1.6479250	-3.1266310
H35	-2.6648540	3.3108470	-2.7617910
H36	-2.4343880	2.0384510	-1.5475680
C37	0.4939470	0.5840220	-6.4012590
H38	0.6731340	-0.4920620	-6.2753020
H39	1.3292120	0.9838710	-6.9854010
H40	-0.4220650	0.6922850	-6.9910510
C41	2.6299560	3.6506700	2.2622840
H42	3.4867020	3.7464220	2.9350370
H43	2.5290270	4.5968050	1.7175230
H44	2.8583370	2.8746630	1.5233420
C45	-2.3473600	2.5999090	2.4326330
H46	-2.6674780	3.5117640	1.9134600
H47	-3.1224670	2.3448120	3.1614130
H48	-2.3000130	1.8016880	1.6847140

C49	0.3970890	2.6593550	6.6825850
H50	1.0318300	3.4288150	7.1361150
H51	0.8394640	1.6877040	6.9378920
H52	-0.5883190	2.7067680	7.1558100
H53	1.1983790	0.8000930	2.4704230
N54	0.8964200	-1.8644230	-0.2305780
C55	1.3565500	-4.5603730	-0.7740200
C56	1.5420770	-2.2464750	-1.3508250
C57	0.4691130	-2.8085090	0.6363290
C58	0.6974240	-4.1666300	0.3873090
C59	1.7861710	-3.5776250	-1.6665430
H60	1.8840920	-1.4457340	-1.9983770
H61	0.3507750	-4.9022370	1.1075100
H62	2.3085130	-3.8296240	-2.5842940
H63	1.5350380	-5.6129510	-0.9775150
C64	-0.2874810	-2.3576300	1.8616830
H65	-0.4140700	-3.2107070	2.5359680
H66	-1.2845500	-2.0390700	1.5389100
C67	0.3757040	-1.2023570	2.6231850
H68	1.3138830	-1.5397880	3.0974370
H69	-0.2689510	-0.9079640	3.4669460
C170	-1.8467430	-0.1455390	-0.2249320

	U	Cv	S	H	G
trans.	0.889	2.981	45.045	1.481	-11.949
rot.	0.889	2.981	37.203	0.889	-10.203
vib.	18.790	120.323	120.645	18.790	-17.181
elec.	0.000	0.000	0.000	0.000	0.000
total	20.567	126.284	202.893	21.160	-39.333

Total internal energy, Utot (SCFE + ZPE + U): -2304.186275 hartrees
Total enthalpy, Htot (Utot + pV): -2304.185331 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2304.281733 hartrees



benzene

Ru1	0.7035374	0.3034762	0.0560744
C12	3.0664496	0.9731521	0.0887691
C3	0.3057765	2.3406287	0.0081856
N4	0.2789817	3.2842505	0.9825463
N5	0.2874598	2.9825253	-1.1897533
C6	0.3537755	4.6651264	0.4489885
H7	-0.4481130	5.2821696	0.8651984
H8	1.3114420	5.1184566	0.7259406
C9	0.2253871	4.4549263	-1.0663810
H10	1.0396361	4.9220281	-1.6271055
H11	-0.7225095	4.8296708	-1.4704964
C12	0.7314601	0.0306805	1.8599909

C113	1.4270037	-1.8391920	-0.8670669
C14	0.1120891	3.1064253	2.3991414
C15	-0.2857721	2.8432505	5.1715233
C16	1.2271001	3.1025443	3.2602657
C17	-1.2001302	3.0706949	2.9157964
C18	-1.3744670	2.9273177	4.2963223
C19	0.9996887	2.9516322	4.6341751
H20	-2.3855399	2.8880920	4.6967745
H21	1.8585908	2.9290179	5.3020394
C22	0.1155908	2.3739517	-2.4839889
C23	-0.2725458	1.2890639	-5.0496057
C24	-1.1883309	2.0414435	-2.9113325
C25	1.2185076	2.2403662	-3.3537006
C26	0.9972774	1.6811756	-4.6182282
C27	-1.3551684	1.4938760	-4.1873229
H28	1.8466355	1.5588174	-5.2869236
H29	-2.3582280	1.2322487	-4.5188190
C30	2.5998235	2.7133710	-2.9748860
H31	2.9215079	2.2889886	-2.0195057
H32	2.6332855	3.8069088	-2.8823977
H33	3.3240671	2.4282114	-3.7428344
C34	-2.3968173	2.2890944	-2.0375677
H35	-3.3123948	1.9902217	-2.5550707
H36	-2.4961896	3.3489392	-1.7772170
H37	-2.3424122	1.7291082	-1.1002161
C38	-0.4697875	0.6597607	-6.4092690
H39	-0.3102701	-0.4249776	-6.3654476
H40	0.2372844	1.0602480	-7.1426607
H41	-1.4842183	0.8258327	-6.7854681
C42	2.6322776	3.3024839	2.7506104
H43	3.3612602	3.0575482	3.5284466
H44	2.7973067	4.3517941	2.4716132
H45	2.8427799	2.6860002	1.8725105
C46	-2.4079113	3.2323969	2.0180088
H47	-2.4923927	4.2615943	1.6455546
H48	-3.3290031	3.0106298	2.5641959
H49	-2.3647945	2.5806894	1.1412468
C50	-0.4915805	2.6395986	6.6548879
H51	0.2890075	3.1364450	7.2397855
H52	-0.4595175	1.5735678	6.9136165
H53	-1.4619755	3.0249955	6.9822865
H54	1.6920712	0.2116731	2.3580931
N55	-1.2677822	-0.5659812	-0.1381137
C56	-3.5687979	-2.0852596	-0.6245332
C57	-1.5894639	-0.9790794	-1.3850900
C58	-2.0847140	-0.9097968	0.8850533
C59	-3.2365394	-1.6729771	0.6612490
C60	-2.7256506	-1.7224401	-1.6725654
H61	-0.8953180	-0.7065384	-2.1689283
H62	-3.8622112	-1.9380490	1.5079662
H63	-2.9251727	-2.0216452	-2.6961958
H64	-4.4598383	-2.6808805	-0.8026810
C65	-1.7596147	-0.4313572	2.2765171
H66	-2.4238391	-0.9400040	2.9824470
H67	-1.9962398	0.6354264	2.3399473
C68	-0.3051263	-0.6156597	2.7218520
H69	-0.0496844	-1.6875678	2.7786692

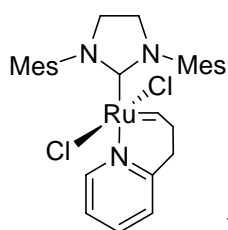
H70 -0.2004974 -0.2338852 3.7470437

	U	Cv	S	H	G
	-----	-----	-----	-----	-----
trans.	0.933	2.981	45.289	1.556	-12.626
rot.	0.933	2.981	37.203	0.933	-10.717
vib.	20.404	125.555	125.192	20.404	-18.800
elec.	0.000	0.000	0.000	0.000	0.000
total	22.271	131.517	207.684	22.893	-42.143

Total internal energy, Utot (SCFE + ZPE + U): -2304.211894 hartrees

Total enthalpy, Htot (Utot + pV): -2304.210902 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -2304.314544 hartrees



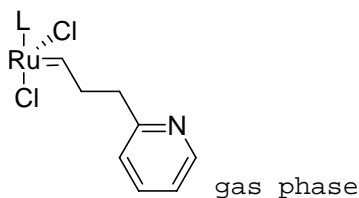
benzene

Ru1	0.5373560	0.3052120	0.0652490
Cl2	2.9299290	0.6613540	-0.3239590
C3	0.2032370	2.3615740	0.0009510
N4	0.0710950	3.2896740	0.9780830
N5	0.0846550	3.0094430	-1.1893860
C6	-0.2161120	4.6495340	0.4644230
H7	-1.2288550	4.9533400	0.7532340
H8	0.4862560	5.3754170	0.8845500
C9	-0.0615070	4.4741650	-1.0521570
H10	0.8282350	4.9786670	-1.4454230
H11	-0.9303240	4.8297740	-1.6132900
C12	0.7462400	0.0454910	1.8595310
C13	0.1359460	3.0965300	2.3985960
C14	0.2735380	2.8194780	5.1875640
C15	1.3701460	3.2897150	3.0528570
C16	-1.0322660	2.7886540	3.1164860
C17	-0.9357940	2.6513060	4.5081120
C18	1.4142020	3.1437400	4.4421430
H19	-1.8340910	2.4080320	5.0722750
H20	2.3650160	3.2827390	4.9538150
C21	0.1899510	2.4205660	-2.5003050
C22	0.3721080	1.2436700	-5.0464570
C23	-0.9865850	1.9873210	-3.1537480
C24	1.4338480	2.3917850	-3.1628060
C25	1.5003330	1.7779310	-4.4210210
C26	-0.8657230	1.3875720	-4.4095860
H27	2.4635120	1.7303020	-4.9257670
H28	-1.7664240	1.0345040	-4.9079030
C29	2.6608410	3.0820220	-2.6150120
H30	3.5720080	2.5960120	-2.9750020
H31	2.6917490	3.0712220	-1.5260420

H32	2.6868760	4.1257330	-2.9606440
C33	-2.3552680	2.2250910	-2.5623130
H34	-3.1295520	1.8129230	-3.2144660
H35	-2.5535670	3.2984730	-2.4539150
H36	-2.4568770	1.7604850	-1.5803730
C37	0.4749560	0.5404360	-6.3804050
H38	0.4709530	-0.5495100	-6.2512140
H39	1.3981670	0.8046310	-6.9046950
H40	-0.3709730	0.7886060	-7.0304850
C41	2.6281280	3.6043780	2.2771200
H42	3.4797380	3.7138720	2.9542570
H43	2.5352210	4.5367760	1.7080770
H44	2.8625170	2.8110630	1.5579940
C45	-2.3579710	2.5928080	2.4207880
H46	-2.6592140	3.4872780	1.8625330
H47	-3.1449050	2.3778080	3.1493300
H48	-2.3149370	1.7647450	1.7050640
C49	0.3605020	2.6485250	6.6872460
H50	0.8843550	3.4891830	7.1557940
H51	0.9160440	1.7397160	6.9503110
H52	-0.6320010	2.5732340	7.1408720
H53	1.2325360	0.8150010	2.4663300
N54	0.9038830	-1.8564840	-0.2310580
C55	1.3500880	-4.5460790	-0.8060000
C56	1.5308500	-2.2278800	-1.3635360
C57	0.4943040	-2.8057690	0.6365680
C58	0.7136800	-4.1616260	0.3704900
C59	1.7679730	-3.5565740	-1.6946530
H60	1.8649530	-1.4202560	-2.0059350
H61	0.3794730	-4.9028050	1.0901780
H62	2.2784590	-3.7995930	-2.6210550
H63	1.5219060	-5.5971530	-1.0222330
C64	-0.2260820	-2.3605240	1.8851140
H65	-0.3310080	-3.2161220	2.5603550
H66	-1.2323640	-2.0408160	1.5944820
C67	0.4595860	-1.2061990	2.6286320
H68	1.4200030	-1.5388990	3.0595030
H69	-0.1539500	-0.9234680	3.4985450
C170	-1.8549880	-0.1806890	-0.1288510

	U	Cv	S	H	G
	-----	-----	-----	-----	-----
trans.	0.933	2.981	45.289	1.556	-12.626
rot.	0.933	2.981	37.346	0.933	-10.761
vib.	20.634	125.776	126.644	20.634	-19.025
elec.	0.000	0.000	0.000	0.000	0.000
total	22.501	131.738	209.278	23.123	-42.412

Total internal energy, Utot (SCFE + ZPE + U): -2304.206111 hartrees
 Total enthalpy, Htot (Utot + pV): -2304.205120 hartrees
 Total Gibbs free energy, Gtot (Htot - T*S): -2304.309557 hartrees

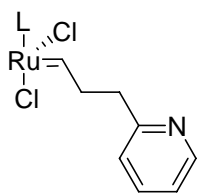


Ru1	0.0000000	0.0000000	0.0000000
Cl2	0.0000000	0.0000000	2.3586860
C3	2.0373800	0.0000000	-0.0377540
N4	2.9468510	0.9885670	-0.1448750
N5	2.6804310	-1.1872860	-0.0061580
C6	4.3412480	0.4755280	-0.1899880
H7	4.8485490	0.8306300	-1.0916380
H8	4.9013670	0.8337690	0.6792870
C9	4.1469430	-1.0533240	-0.1790260
H10	4.6806730	-1.5411090	0.6408590
H11	4.4571730	-1.5276140	-1.1165950
Cl12	-0.3224300	1.7627710	-0.3246230
Cl13	-2.1876750	-0.9832680	-0.3785960
C14	2.6827800	2.3995400	-0.1691400
C15	2.1276420	5.1482970	-0.2236310
C16	2.6681790	3.1221240	1.0394080
C17	2.4787570	3.0382460	-1.4082810
C18	2.1967220	4.4087100	-1.4098560
C19	2.3887200	4.4924260	0.9856710
H20	2.0150890	4.9063810	-2.3606080
H21	2.3576430	5.0569610	1.9155200
C22	2.0362860	-2.4748120	0.0353280
C23	0.8774920	-5.0341250	0.0983470
C24	1.4956160	-3.0218100	-1.1469990
C25	2.0253070	-3.2008150	1.2455860
C26	1.4405010	-4.4710620	1.2495030
C27	0.9171970	-4.2950520	-1.0884100
H28	1.4259990	-5.0364280	2.1796700
H29	0.4972900	-4.7225640	-1.9970790
C30	2.6300400	-2.6443940	2.5128700
H31	2.2140870	-1.6599450	2.7451790
H32	3.7187010	-2.5367940	2.4339340
H33	2.4272780	-3.3094520	3.3571920
C34	1.5360620	-2.2744360	-2.4609290
H35	1.2522090	-2.9324590	-3.2870150
H36	2.5306800	-1.8694440	-2.6752000
H37	0.8353440	-1.4290180	-2.4643810
C38	0.2358920	-6.4021790	0.1423900
H39	-0.8248590	-6.3295330	0.4134750
H40	0.7162300	-7.0451170	0.8869280
H41	0.2887830	-6.9016190	-0.8301160
C42	2.9117410	2.4466150	2.3677720
H43	2.8627180	3.1749190	3.1820910
H44	3.8971790	1.9676890	2.4087480
H45	2.1626300	1.6709800	2.5581650
C46	2.5410350	2.2728620	-2.7105740
H47	3.5492030	1.8879030	-2.9072640
H48	2.2629570	2.9159320	-3.5501260
H49	1.8652380	1.4101470	-2.7098910

C50	1.7225880	6.6032360	-0.2398170
H51	2.1913690	7.1621810	0.5762910
H52	0.6348000	6.6870240	-0.1151400
H53	1.9856740	7.0853280	-1.1864590
H54	-0.1371280	2.0510980	-1.3769990
N55	-2.2233790	5.7230000	0.6267150
C56	-4.5767440	5.3365170	2.0936170
C57	-2.7617390	6.7100230	1.3582380
C58	-2.8487840	4.5305510	0.6145360
C59	-4.0279740	4.3025260	1.3363340
C60	-3.9305780	6.5724240	2.1076860
H61	-2.2341120	7.6627280	1.3405900
H62	-4.5099900	3.3307380	1.2958630
H63	-4.3195250	7.4111030	2.6780210
H64	-5.4931300	5.1799480	2.6573500
C65	-2.2123290	3.4320230	-0.2118560
H66	-1.8998150	3.8481190	-1.1764490
H67	-2.9470720	2.6443260	-0.4083290
C68	-0.9748310	2.8202590	0.5026900
H69	-1.2493650	2.4323930	1.4860520
H70	-0.2402580	3.6252140	0.6568310

	U	Cv	S	H	G
trans.	0.889	2.981	45.045	1.481	-11.949
rot.	0.889	2.981	37.613	0.889	-10.326
vib.	19.594	122.086	130.265	19.594	-19.245
elec.	0.000	0.000	0.000	0.000	0.000
total	21.371	128.048	212.923	21.964	-41.519

Total internal energy, Utot (SCFE + ZPE + U): -2304.148685 hartrees
Total enthalpy, Htot (Utot + pV): -2304.147741 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2304.248908 hartrees



methylene chloride

Ru1	0.0000000	0.0000000	0.0000000
Cl2	2.3586860	0.0000000	0.0000000
C3	-0.0377540	2.0373800	0.0000000
N4	-0.1448750	2.9468510	0.9885670
N5	-0.0061580	2.6804310	-1.1872860
C6	-0.1899880	4.3412480	0.4755280
H7	-1.0916380	4.8485490	0.8306300
H8	0.6792870	4.9013670	0.8337690
C9	-0.1790260	4.1469430	-1.0533240
H10	0.6408590	4.6806730	-1.5411090
H11	-1.1165950	4.4571730	-1.5276140
C12	-0.3246230	-0.3224300	1.7627710

C113	-0.3785960	-2.1876750	-0.9832680
C14	-0.1691400	2.6827800	2.3995400
C15	-0.2236310	2.1276420	5.1482970
C16	1.0394080	2.6681790	3.1221240
C17	-1.4082810	2.4787570	3.0382460
C18	-1.4098560	2.1967220	4.4087100
C19	0.9856710	2.3887200	4.4924260
H20	-2.3606080	2.0150890	4.9063810
H21	1.9155200	2.3576430	5.0569610
C22	0.0353280	2.0362860	-2.4748120
C23	0.0983470	0.8774920	-5.0341250
C24	-1.1469990	1.4956160	-3.0218100
C25	1.2455860	2.0253070	-3.2008150
C26	1.2495030	1.4405010	-4.4710620
C27	-1.0884100	0.9171970	-4.2950520
H28	2.1796700	1.4259990	-5.0364280
H29	-1.9970790	0.4972900	-4.7225640
C30	2.5128700	2.6300400	-2.6443940
H31	2.7451790	2.2140870	-1.6599450
H32	2.4339340	3.7187010	-2.5367940
H33	3.3571920	2.4272780	-3.3094520
C34	-2.4609290	1.5360620	-2.2744360
H35	-3.2870150	1.2522090	-2.9324590
H36	-2.6752000	2.5306800	-1.8694440
H37	-2.4643810	0.8353440	-1.4290180
C38	0.1423900	0.2358920	-6.4021790
H39	0.4134750	-0.8248590	-6.3295330
H40	0.8869280	0.7162300	-7.0451170
H41	-0.8301160	0.2887830	-6.9016190
C42	2.3677720	2.9117410	2.4466150
H43	3.1820910	2.8627180	3.1749190
H44	2.4087480	3.8971790	1.9676890
H45	2.5581650	2.1626300	1.6709800
C46	-2.7105740	2.5410350	2.2728620
H47	-2.9072640	3.5492030	1.8879030
H48	-3.5501260	2.2629570	2.9159320
H49	-2.7098910	1.8652380	1.4101470
C50	-0.2398170	1.7225880	6.6032360
H51	0.5762910	2.1913690	7.1621810
H52	-0.1151400	0.6348000	6.6870240
H53	-1.1864590	1.9856740	7.0853280
H54	-1.3769990	-0.1371280	2.0510980
N55	0.6267150	-2.2233790	5.7230000
C56	2.0936170	-4.5767440	5.3365170
C57	1.3582380	-2.7617390	6.7100230
C58	0.6145360	-2.8487840	4.5305510
C59	1.3363340	-4.0279740	4.3025260
C60	2.1076860	-3.9305780	6.5724240
H61	1.3405900	-2.2341120	7.6627280
H62	1.2958630	-4.5099900	3.3307380
H63	2.6780210	-4.3195250	7.4111030
H64	2.6573500	-5.4931300	5.1799480
C65	-0.2118560	-2.2123290	3.4320230
H66	-1.1764490	-1.8998150	3.8481190
H67	-0.4083290	-2.9470720	2.6443260
C68	0.5026900	-0.9748310	2.8202590
H69	1.4860520	-1.2493650	2.4323930

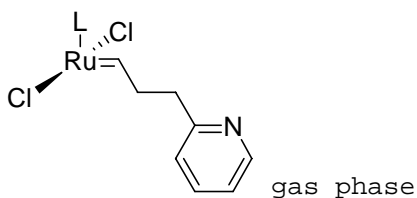
H70 0.6568310 -0.2402580 3.6252140

	U	Cv	S	H	G
-----	-----	-----	-----	-----	-----
trans.	0.889	2.981	45.045	1.481	-11.949
rot.	0.889	2.981	37.631	0.889	-10.331
vib.	19.523	122.031	129.351	19.523	-19.043
elec.	0.000	0.000	0.000	0.000	0.000
total	21.301	127.992	212.027	21.893	-41.323

Total internal energy, Utot (SCFE + ZPE + U): -2304.221121 hartrees

Total enthalpy, Htot (Utot + pV): -2304.220177 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -2304.320918 hartrees

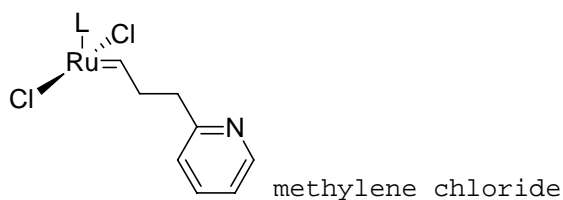


Ru1	0.4062136	0.5698522	0.4825423
Cl2	2.7404720	0.3200828	0.0783597
C3	0.3307903	2.5067492	0.0915826
N4	0.3622605	3.5782638	0.9240182
N5	0.2963848	2.9777886	-1.1863158
C6	0.2701300	4.8661351	0.2060179
H7	-0.7016150	5.3368370	0.3990914
H8	1.0517524	5.5499694	0.5490675
C9	0.4406616	4.4442650	-1.2583856
H10	1.4288214	4.7040792	-1.6568045
H11	-0.3179142	4.8725937	-1.9194920
Cl2	0.4206386	0.4462199	2.2947361
Cl3	0.3384220	3.5904488	2.3569682
Cl4	0.3090405	3.6809467	5.1556829
Cl5	1.5584577	3.6721184	3.0544073
Cl6	-0.8957638	3.5676222	3.0295546
Cl7	-0.8827637	3.6144066	4.4283817
Cl8	1.5172726	3.7146430	4.4504542
H19	-1.8307009	3.5887912	4.9612530
H20	2.4541971	3.7666838	5.0006991
C21	0.2354642	2.2149759	-2.4074420
C22	0.0713736	0.8298497	-4.8417312
C23	-1.0328029	1.9518384	-2.9729175
C24	1.4196802	1.8832415	-3.0927940
C25	1.3077691	1.1728823	-4.2943637
C26	-1.0868204	1.2475737	-4.1764531
H27	2.2189779	0.8969236	-4.8206922
H28	-2.0596900	1.0320284	-4.6122663
C29	2.7844668	2.3428335	-2.6383967
H30	3.5479870	1.6085897	-2.9074600
H31	2.8413302	2.4855875	-1.5604734
H32	3.0477049	3.2862258	-3.1364672

C33	-2.3056054	2.4574943	-2.3375068
H34	-3.1598915	2.2608952	-2.9909237
H35	-2.2650351	3.5393373	-2.1623104
H36	-2.4926395	1.9679423	-1.3787717
C37	-0.0211502	0.0389405	-6.1251968
H38	-0.1881985	-1.0251172	-5.9181011
H39	0.8980600	0.1184919	-6.7129077
H40	-0.8547113	0.3816210	-6.7471065
C41	2.8800538	3.6667386	2.3236607
H42	3.7102219	3.7476159	3.0300538
H43	2.9611511	4.5027635	1.6189465
H44	3.0103383	2.7445350	1.7467819
C45	-2.2015913	3.4389547	2.2814449
H46	-2.3377099	4.2407375	1.5469342
H47	-3.0450383	3.4811502	2.9751303
H48	-2.2560817	2.4895161	1.7368948
C49	0.3006467	3.6864899	6.6665689
H50	1.0386240	4.3883004	7.0683943
H51	0.5493549	2.6946126	7.0637947
H52	-0.6812999	3.9619964	7.0613261
H53	0.3886897	1.2681466	3.0099118
N54	0.1472034	-2.8301035	5.2891728
C55	-1.4458110	-4.9277035	4.3463646
C56	0.2488460	-4.0634510	5.7954849
C57	-0.7485317	-2.6227401	4.3089359
C58	-1.5638746	-3.6469025	3.8103185
C59	-0.5186157	-5.1459052	5.3634134
H60	0.9836415	-4.1947654	6.5887864
H61	-2.2722260	-3.4367524	3.0144020
H62	-0.3893262	-6.1263287	5.8115501
H63	-2.0658718	-5.7394070	3.9752205
C64	-0.8019069	-1.2264404	3.7320291
H65	-0.8336448	-0.4995101	4.5514559
H66	-1.7012060	-1.0964383	3.1225772
C67	0.4492979	-0.9409037	2.8574071
H68	0.5176692	-1.6972883	2.0623999
H69	1.3495305	-1.0559827	3.4797186
C170	-1.8935274	0.0149145	0.1288734

	U	Cv	S	H	G
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trans.	0.889	2.981	45.045	1.481	-11.949
rot.	0.889	2.981	37.791	0.889	-10.379
vib.	19.349	121.378	129.127	19.349	-19.150
elec.	0.000	0.000	0.000	0.000	0.000
total	21.127	127.339	211.963	21.719	-41.478

Total internal energy, Utot (SCFE + ZPE + U): -2304.161722 hartrees
 Total enthalpy, Htot (Utot + pV): -2304.160778 hartrees
 Total Gibbs free energy, Gtot (Htot - T*S): -2304.261489 hartrees



Ru1	0.3951405	0.5223240	0.3534278
Cl2	2.7704853	0.3964494	-0.0473932
C3	0.2584949	2.4939512	0.0756961
N4	0.1862724	3.5260843	0.9460253
N5	0.1709102	2.9951292	-1.1848184
C6	-0.0041792	4.8350949	0.2723907
H7	-0.9782533	5.2557217	0.5425226
H8	0.7699313	5.5400843	0.5893984
C9	0.0907074	4.4724714	-1.2171728
H10	0.9841346	4.8868765	-1.6959802
H11	-0.7845746	4.7950456	-1.7879234
Cl2	0.4951203	0.3293785	2.1624002
Cl3	0.2740031	3.5046965	2.3785410
Cl4	0.4571845	3.5673576	5.1765106
Cl5	1.5406694	3.6282350	2.9838413
Cl6	-0.9035962	3.4380184	3.1450811
Cl7	-0.7848158	3.4659651	4.5407215
Cl8	1.6063127	3.6531617	4.3806105
H19	-1.6890578	3.4071114	5.1438111
H20	2.5806036	3.7436588	4.8580852
C21	0.2587275	2.2527885	-2.4170685
C22	0.4109795	0.8389414	-4.8424760
C23	-0.9318486	1.8445229	-3.0614020
C24	1.5133879	2.0686309	-3.0345753
C25	1.5626316	1.3428348	-4.2315278
C26	-0.8275188	1.1215776	-4.2539368
H27	2.5306798	1.1809266	-4.7026317
H28	-1.7404412	0.7885911	-4.7445566
C29	2.7764514	2.7137170	-2.5135092
H30	3.6566230	2.1294613	-2.7952706
H31	2.7772151	2.8151041	-1.4290288
H32	2.8939533	3.7136215	-2.9538252
C33	-2.2949863	2.2596201	-2.5603056
H34	-3.0792863	1.6712778	-3.0448409
H35	-2.4835725	3.3142307	-2.8021915
H36	-2.3946818	2.1361710	-1.4822597
C37	0.4946292	0.0182127	-6.1088864
H38	0.4907511	-1.0550890	-5.8789448
H39	1.4128538	0.2296132	-6.6654243
H40	-0.3592169	0.2093014	-6.7674647
C41	2.8034769	3.7136746	2.1586867
H42	3.6759766	3.8455646	2.8046701
H43	2.7758835	4.5574752	1.4591486
H44	2.9551813	2.8060843	1.5640735
C45	-2.2638508	3.3231629	2.4976145
H46	-2.5221816	4.2285729	1.9342200
H47	-3.0379848	3.1781623	3.2563447
H48	-2.3067925	2.4810987	1.7993872
C49	0.5648210	3.5688594	6.6845532

H50	1.3402147	4.2617622	7.0283204
H51	0.8330351	2.5733864	7.0615519
H52	-0.3816094	3.8532595	7.1539775
H53	0.5833442	1.1478324	2.8795492
N54	0.4324784	-3.2323372	4.7549930
C55	-2.0464060	-4.4865091	5.0765630
C56	0.3385933	-4.4762238	5.2480237
C57	-0.7023332	-2.5956199	4.4133923
C58	-1.9611344	-3.1938162	4.5597665
C59	-0.8702773	-5.1473112	5.4304887
H60	1.2785134	-4.9599904	5.5116684
H61	-2.8565583	-2.6485401	4.2743215
H62	-0.8828308	-6.1550537	5.8360464
H63	-3.0129421	-4.9685697	5.1997166
C64	-0.5705178	-1.1803214	3.8838398
H65	-0.2625957	-0.5169267	4.7029978
H66	-1.5486821	-0.8330793	3.5375827
C67	0.4647682	-1.0549415	2.7355940
H68	0.2567107	-1.8064137	1.9634118
H69	1.4632688	-1.2900420	3.1337626
C170	-1.9735605	0.1519966	0.1379206

	U	Cv	S	H	G
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trans.	0.933	2.981	45.289	1.556	-12.626
rot.	0.933	2.981	37.967	0.933	-10.956
vib.	21.205	126.688	135.812	21.205	-21.324
elec.	0.000	0.000	0.000	0.000	0.000
total	23.072	132.650	219.067	23.694	-44.906

Total internal energy, Utot (SCFE + ZPE + U): -2304.219344 hartrees
 Total enthalpy, Htot (Utot + pV): -2304.218353 hartrees
 Total Gibbs free energy, Gtot (Htot - T*S): -2304.327675 hartrees